Theory of screening of the phonon-modulated spin-orbit interaction in metals

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We investigate the long-wavelength limit of the phonon-modulated spin-orbit interaction in the self-consistent Hartree approximation. Within the jellium model we show that the screening is provided by the spin-other-orbits term in the electron-electron interaction. In the case of a discrete-lattice model, the modifications in the electronic wave functions induced by the spin-orbit coupling of the electrons to the ions give rise to spin-mixed matrix elements of the Coulomb electron-electron interaction. This is able to provide a further screening mechanism to the phonon-modulated spin-orbit interaction. Our self-consistent treatment of the screening justifies *a posteriori* the results of previous theories based on an already screened lattice potential. [S0163-1829(97)04520-7]

I. INTRODUCTION

The spin-orbit coupling of the conduction electrons to the lattice potential can be modulated by lattice vibrations. This leads to an interaction in which the spin of the electron is coupled to the quantum of the lattice vibrations (phonon). This phonon-modulated spin-orbit interaction (PMSOI) influences the lifetime of the electron-spin orientation, and has consequences for spin-polarized transport; a field which has recently gained great interest because of possible device applications.[1]

The important role of spin-orbit interaction in electron-phonon scattering in metals was pointed out in 1953 by Overhauser,[2] who made use of a simple jellium model in his calculations. A new approach to this problem was introduced one year later by Elliott,[3] who used a more realistic set of electronic wave functions than simple plane waves. Both procedures, however, showed a strong model dependence, leading, for example, to different temperature dependences of the calculated spin-relaxation times of the electrons. In 1963, Yafet[4] was able to reconcile the previous approaches in a single theory by making use of simple theorems on the spin symmetry of the Hamiltonian. The main consequence of his theory is that the matrix element of the spin-reversal interaction due to lattice vibrations, $M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}$, is proportional to q^2 for small momentum transfer $\mathbf{q}$. This determines the low-temperature behavior of the inverse of the longitudinal electron spin-relaxation time T_1^{-1}, which results to be proportional to T^5 for temperatures well below the Debye temperature T_D. On the other hand for $T \gg T_D$ the details of the matrix element are not essential, and $T_1^{-1} \propto T$. Therefore, the calculated temperature dependence of T_1^{-1} is very similar to the one observed in the resistivity ρ. This led to the establishment of a simple relation known as the Elliott-Yafet formula:[3,4] $T_1^{-1} \propto (\Delta g)^2 \rho$, where Δg is the shift of the g factor due to the spin-orbit coupling of the electrons to the lattice potential.

Experimentally, at low temperatures, a T^5 dependence of T_1^{-1} is observed in many metals by making use of different techniques,[5] and the behavior predicted by the Elliott-Yafet formula was confirmed for a wide range of temperatures. On the other hand, all the theoretical results were based on the assumption of an *a priori* screened lattice potential. What remained unclear is the physical process of screening of the PMSOI and the main purpose of this paper is to clear up this point. Indeed, screening of the PMSOI should be considered separately from the one occurring in the ordinary electron-phonon interaction (EPI). If we start from bare EPI and PMSOI matrix elements, then corresponding screened quantities are obtained by considering the response of the conduction electrons to the lattice distortion. It is straightforward to show that, when the electron-electron interaction is given just by the Coulomb repulsion, the conduction electrons screen the EPI, while the PMSOI remains unscreened. This is due to the fact that the Coulomb interaction conserves the electron-spin orientation, whereas the PMSOI is a spin-dependent interaction. However, the PMSOI is a relativistic effect, and it is plausible to search for the mechanism of its screening by considering the relativistic corrections to the electron-electron interaction. This is done in Sec. II, where we calculate the bare PMSOI matrix element for the jellium model and determine, in the Hartree approximation, the corresponding screened matrix element. In Sec. III we extend our analysis to a more realistic model in which the lattice structure is taken into account.

II. JELLIUM MODEL

A. Hartree approximation

In the jellium model, the discrete nature of the lattice is replaced by a continuum of positive charge in which the electrons are embedded. The infinite electrostatic potential given by a uniform distribution of the positive charge is canceled by the electrostatic contribution of the electrons in order to preserve the charge neutrality of the system. Fluctuations of the positive charge density lead to the following change in the electrostatic potential:

$$\delta W(\mathbf{r}) = -Z_c e^2 n_o \int d^3r' \frac{\nabla\cdot\mathbf{u}(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \tag{1}$$

where $Z_c e n_o$ is the charge density of a unit cell, and $\mathbf{u}(\mathbf{r})$ is the displacement vector. The spin-orbit interaction associated with the potential (1) is given by

$$\delta W_{s\text{-}o}(\mathbf{r}) = \frac{\hbar}{4m^2c^2}\boldsymbol{\nabla}_{\mathbf{r}}\delta W(\mathbf{r})\times\mathbf{p}\cdot\boldsymbol{\sigma}. \tag{2}$$

Here m is the mass of the electron, and c is the speed of light. $\mathbf{p}=-i\hbar\boldsymbol{\nabla}$ and $\boldsymbol{\sigma}$ are the electronic momentum and spin operators, respectively. When $\mathbf{u}(\mathbf{r})$ is expressed in normal coordinates, Eqs. (1) and (2) give rise to the usual bare EPI and the bare PMSOI, respectively.

Until here, the potentials in Eqs. (1) and (2) have been the bare ones. In order to include screening, we have to consider also the electron-electron interaction. Therefore we introduce the following electronic Hamiltonian:

$$H=\sum_i \left[\frac{p_i^2}{2m}+\delta W(\mathbf{r}_i)+\delta W_{s\text{-}o}(\mathbf{r}_i)\right]+\tfrac{1}{2}\sum_{i\neq j} V_{i,j}^{e\text{-}e}. \tag{3}$$

Here $V_{i,j}^{e\text{-}e}$ is the electron-electron interaction potential. When $V_{i,j}^{e\text{-}e}$ is given just by the Coulomb repulsion $V_{i,j}^{c}=e^2/r_{ij}$ with $r_{ij}=|\mathbf{r}_i-\mathbf{r}_j|$, then the response of the electrons to potential (1) leads to a screened electron-jellium interaction, $\delta\widehat{W}(\mathbf{r})$, and the associated EPI becomes short ranged.[6] In Ref. 2, the screened spin-orbit potential, $\delta\widehat{W}_{s\text{-}o}(\mathbf{r})$, was obtained by replacing in Eq. (2) the bare $\delta W(\mathbf{r})$ by the screened one $\delta\widehat{W}(\mathbf{r})$.[7] However, when we follow a self-consistent treatment of the electronic response to the perturbation (2), we find that the PMSOI remains unscreened. This is due to the fact that, unlike $\delta W(\mathbf{r})$, the spin-orbit potential (2) does not couple to the electron density because of the presence of the spin operator. This can be readily seen when we employ the Hartree approximation. In this case, Eq. (3) reduces to the one-electron Hamiltonian

$$H_H=\frac{p^2}{2m}+\delta W(\mathbf{r})+\delta W_{s\text{-}o}(\mathbf{r})+V_H^c(\mathbf{r}), \tag{4}$$

where $V_H^c(\mathbf{r})$ is the Coulomb potential in the Hartree approximation,

$$V_H^c(\mathbf{r})=e^2\int d^3r'\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \tag{5}$$

In the above equation, $\rho(\mathbf{r})=\Sigma_{\mathbf{k},\sigma}^{(\mathrm{occ.})}|\psi_{\mathbf{k},\sigma}(\mathbf{r})|^2$ is the electronic density (the summation is performed over the occupied states), and $\psi_{\mathbf{k},\sigma}(\mathbf{r})$ is the single-electron eigenfunction solution of Eq. (4).

We follow the common procedure[6] in evaluating the response of the electrons to the perturbation potentials $\delta W(\mathbf{r})$ and $\delta W_{s\text{-}o}(\mathbf{r})$. For a homogeneous positive charge density, the potentials $\delta W(\mathbf{r})$ and $\delta W_{s\text{-}o}(\mathbf{r})$ are zero and the electronic density is $\rho_0(\mathbf{r})=\Sigma_{\mathbf{k},\sigma}^{(\mathrm{occ.})}|\phi_{\mathbf{k},\sigma}(\mathbf{r})|^2$, where $\phi_{\mathbf{k},\sigma}(\mathbf{r})$ is a plane wave with eigenvalues $\epsilon_{\mathbf{k}}$. In the presence of the perturbation potentials $\delta W(\mathbf{r})$ and $\delta W_{s\text{-}o}(\mathbf{r})$ the electronic wave functions are modified as $\psi_{\mathbf{k},\sigma}(\mathbf{r})=\phi_{\mathbf{k},\sigma}(\mathbf{r})+\delta\phi_{\mathbf{k},\sigma}(\mathbf{r})$ and consequently the electronic density takes the form $\rho(\mathbf{r})=\rho_0(\mathbf{r})+\delta\rho(\mathbf{r})$, where

$$\delta\rho(\mathbf{r})=\sum_{\mathbf{k},\sigma}^{(\mathrm{occ.})}\left[\delta\phi_{\mathbf{k},\sigma}^*(\mathbf{r})\phi_{\mathbf{k},\sigma}(\mathbf{r})+\phi_{\mathbf{k},\sigma}^*(\mathbf{r})\delta\phi_{\mathbf{k},\sigma}(\mathbf{r})\right]. \tag{6}$$

The Hamiltonian (4) can therefore be written as

$$H_H=\frac{p^2}{2m}+\delta W(\mathbf{r})+\delta W_{s\text{-}o}(\mathbf{r})+V_{H0}^c(\mathbf{r})+\delta V_H^c(\mathbf{r}). \tag{7}$$

Here $V_{H0}^c(\mathbf{r})$ is the potential given by Eq. (5), where $\rho(\mathbf{r})$ has to be replaced by the unperturbed electronic density $\rho_0(\mathbf{r})$, and $\delta V_H^c(\mathbf{r})$ is the following potential:

$$\delta V_H^c(\mathbf{r})=e^2\int d^3r'\frac{\delta\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}. \tag{8}$$

Now, following Ref. 6, the effective electron-jellium potential $\delta\widehat{W}(\mathbf{r})$ is given by

$$\delta\widehat{W}(\mathbf{r})=\delta W(\mathbf{r})+\delta V_H^c(\mathbf{r})=\delta W(\mathbf{r})+e^2\int d^3r'\frac{\delta\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}, \tag{9}$$

whereas the spin-orbit potential $\delta W_{s\text{-}o}(\mathbf{r})$ remains unaffected by the electronic response. Therefore the inclusion of just the Coulomb repulsion leads to a screened short-range EPI while the PMSOI continues to be long ranged. This means that the replacement of $\delta W(\mathbf{r})$ by $\delta\widehat{W}(\mathbf{r})$ in Eq. (2), as done in Ref. 2, is not justified, and the screening mechanism of the PMSOI remains undetermined.

On the other hand, $\delta W_{s\text{-}o}(\mathbf{r})$ is of order α^2, where α is the fine-structure constant. Therefore, we should consider in the electron-electron interaction $V_{i,j}^{e\text{-}e}$ also the first relativistic corrections to order α^2. These are given by several interaction terms,[8] among which we identified the so-called spin-other-orbits potential $V_{i,j}^{s\text{-}o}$ as the one responsible for the screening of the PMSOI. Following Slater,[8] this relativistic interaction has the following form:

$$V_{i,j}^{s\text{-}o}=\frac{e^2\hbar}{4m^2c^2}\left[\left(\boldsymbol{\nabla}_i\frac{1}{r_{ij}}\right)\times\mathbf{p}_i\cdot\boldsymbol{\sigma}_i+\left(\boldsymbol{\nabla}_j\frac{1}{r_{ij}}\right)\times\mathbf{p}_j\cdot\boldsymbol{\sigma}_j\right]. \tag{10}$$

In our analysis, we are interested only on the mechanisms responsible for the screening of the EPI and the PMSOI. To this end, we consider the Hamiltonian (3) in which the electron-electron interaction is now given by $V_{i,j}^{e\text{-}e}=V_{i,j}^{c}+V_{i,j}^{s\text{-}o}$, where all the other relativistic corrections are neglected. In the following we show that, within the self-consistent Hartree approximation, the spin-other-orbits potential $V_{i,j}^{s\text{-}o}$ together with the Coulomb repulsion in fact provides the correct screening to the PMSOI. The one-electron Hamiltonian is now

$$H_H=\frac{p^2}{2m}+\delta W(\mathbf{r})+\delta W_{s\text{-}o}(\mathbf{r})+V_H^c(\mathbf{r})+V_H^{s\text{-}o}(\mathbf{r}). \tag{11}$$

Here $V_H^c(\mathbf{r})$ is still given by Eq. (5), and $V_H^{s\text{-}o}(\mathbf{r})$ is the spin-other-orbits potential in the Hartree approximation:

$$V_H^{s\text{-}o}(\mathbf{r})=\frac{e^2\hbar}{4m^2c^2}\left\{\left[\nabla_{\mathbf{r}}\int d^3r'\,\frac{\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right]\times\mathbf{p}\cdot\boldsymbol{\sigma}+\sum_{\mathbf{k}',\sigma'}\int d^3r'\,\psi^*_{\mathbf{k}',\sigma'}(\mathbf{r}')\left(\nabla_{\mathbf{r}'}\frac{1}{|\mathbf{r}-\mathbf{r}'|}\right)\times\mathbf{p}'\cdot\boldsymbol{\sigma}\psi_{\mathbf{k}',\sigma'}(\mathbf{r}')\right\}. \tag{12}$$

Here $\psi_{\mathbf{k},\sigma}(\mathbf{r})$ is now the single-electron eigenfunction of Eq. (11).[9]

In Eq. (12), $V_H^{s\text{-}o}(\mathbf{r})$ is given by two terms, of which only the first one contributes significantly to the screening of the PMSOI. In fact, it can be shown that the second term on the right-hand side of Eq. (12) gives corrections of higher order in α^2. Therefore, we shall include in $V_H^{s\text{-}o}(\mathbf{r})$ only the first term of Eq. (12).

We follow the same procedure as above. The response of the electron to the perturbation potentials $\delta W(\mathbf{r})$ and $\delta W_{s\text{-}o}(\mathbf{r})$ leads to the following expression:

$$H_H=\frac{p^2}{2m}+\delta W(\mathbf{r})+\delta W_{s\text{-}o}(\mathbf{r})+V_{H0}^c(\mathbf{r})+\delta V_H^c(\mathbf{r})+V_{H0}^{s\text{-}o}(\mathbf{r})+\delta V_H^{s\text{-}o}(\mathbf{r}). \tag{13}$$

Here $V_{H0}^c(\mathbf{r})$ and $V_{H0}^{s\text{-}o}(\mathbf{r})$ are the potentials given by Eqs. (5) and (12), respectively, where $\rho(\mathbf{r})$ has to be replaced by $\rho_0(\mathbf{r})$. $\delta V_H^c(\mathbf{r})$ is still given by Eq. (8) whereas $\delta V_H^{s\text{-}o}(\mathbf{r})$ reads

$$\delta V_H^{s\text{-}o}(\mathbf{r})=\frac{e^2\hbar}{4m^2c^2}\left[\nabla_{\mathbf{r}}\int d^3r'\,\frac{\delta\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right]\times\mathbf{p}\cdot\boldsymbol{\sigma}. \tag{14}$$

The effective electron-jellium interaction is still given formally by Eq. (9). But now, because of the presence of the spin-other-orbit interaction, we find that also the spin-orbit potential $\delta W_{s\text{-}o}(\mathbf{r})$ is modified by the response of the electrons:

$$\widehat{\delta W}_{s\text{-}o}(\mathbf{r})=\delta W_{s\text{-}o}(\mathbf{r})+\delta V_H^{s\text{-}o}(\mathbf{r})=\delta W_{s\text{-}o}(\mathbf{r})+\frac{e^2\hbar}{4m^2c^2}\left[\nabla_{\mathbf{r}}\int d^3r'\,\frac{\delta\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\right]\times\mathbf{p}\cdot\boldsymbol{\sigma}. \tag{15}$$

Making use of the definition of the bare $\delta W_{s\text{-}o}(\mathbf{r})$ given in Eq. (2) and of the screened electron-jellium potential in Eq. (9), we can rewrite Eq. (15) in the following way:

$$\widehat{\delta W}_{s\text{-}o}(\mathbf{r})=\frac{\hbar}{4m^2c^2}\nabla_{\mathbf{r}}\widehat{\delta W}(\mathbf{r})\times\mathbf{p}\cdot\boldsymbol{\sigma}. \tag{16}$$

This result therefore states that, in order to obtain the screened spin-orbit potential $\widehat{\delta W}_{s\text{-}o}(\mathbf{r})$, the replacement $\delta W(\mathbf{r})\rightarrow\widehat{\delta W}(\mathbf{r})$ is justified only when the spin-other-orbits interaction is taken into account.

B. PMSOI matrix element

An explicit expression of the effective PMSOI matrix element requires the solution of the self-consistent equations given in Eqs. (9) and (15). The variation $\delta\rho(\mathbf{r})$ of the electronic density is calculated by means of Eq. (6), where $\delta\phi_{\mathbf{k},\sigma}(\mathbf{r})$ is the variation of the wave function in the presence of the screened potentials $\widehat{\delta W}(\mathbf{r})$ and $\widehat{\delta W}_{s\text{-}o}(\mathbf{r})$. To lowest order we obtain

$$\delta\phi_{\mathbf{k},\sigma}(\mathbf{r})=\sum_{\mathbf{k}',\sigma'}\frac{\langle\phi_{\mathbf{k}',\sigma'}|\,\widehat{\delta W}(\mathbf{r})+\widehat{\delta W}_{s\text{-}o}(\mathbf{r})\,|\phi_{\mathbf{k},\sigma}\rangle}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}\phi_{\mathbf{k}',\sigma'}(\mathbf{r}). \tag{17}$$

In this way, Eqs. (9) and (15) become

$$\widehat{\delta W}(\mathbf{r})=\delta W(\mathbf{r})+e^2\sum_{\mathbf{k}\mathbf{k}',\sigma}\frac{n_{\mathbf{k}}-n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}\langle\phi_{\mathbf{k}',\sigma}|\,\widehat{\delta W}(\mathbf{r})\,|\phi_{\mathbf{k},\sigma}\rangle\times\langle\phi_{\mathbf{k},\sigma}|\frac{1}{|\mathbf{r}-\mathbf{r}'|}|\phi_{\mathbf{k}',\sigma}\rangle, \tag{18}$$

$$\widehat{\delta W}_{s\text{-}o}(\mathbf{r})=\delta W_{s\text{-}o}(\mathbf{r})+\frac{e^2\hbar}{4m^2c^2}\sum_{\mathbf{k}\mathbf{k}',\sigma}\frac{n_{\mathbf{k}}-n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}}-\epsilon_{\mathbf{k}'}}\langle\phi_{\mathbf{k}',\sigma}|\,\widehat{\delta W}(\mathbf{r})\,|\phi_{\mathbf{k},\sigma}\rangle\times\langle\phi_{\mathbf{k},\sigma}|\nabla_{\mathbf{r}}\frac{1}{|\mathbf{r}-\mathbf{r}'|}|\phi_{\mathbf{k}',\sigma}\rangle\times\frac{\hbar}{i}\nabla_{\mathbf{r}}\cdot\boldsymbol{\sigma}, \tag{19}$$

where $n_{\mathbf{k}}$ is the occupation number of state $\mathbf{k}$. The first equation describes the screening effect of the conduction electrons on the modified jellium potential, while the second one gives the screening of the associated spin-orbit interaction. As already pointed out, when we neglect the spin-other-orbits two-particle interaction, Eq. (10), the second term of the right-hand side of Eq. (19) becomes zero and the spin-orbit potential remains unscreened, i.e., $\widehat{\delta W}_{s\text{-}o}(\mathbf{r})=\delta W_{s\text{-}o}(\mathbf{r})$.

In order to obtain the matrix elements of the EPI and PMSOI, we must express the displacement vector $\mathbf{u}(\mathbf{r})$ appearing in Eqs. (1) and (2) in terms of the normal coordinates

$$\mathbf{u}(\mathbf{r})=\sum_{\mathbf{q}}A_{\mathbf{q}}\hat{\boldsymbol{\epsilon}}_{\mathbf{q}}e^{i\mathbf{q}\cdot\mathbf{r}}. \tag{20}$$

Here $A_{\mathbf{q}}$ is the amplitude of the $\mathbf{q}$ mode, and $\hat{\boldsymbol{\epsilon}}_{\mathbf{q}}$ is the corresponding polarization vector. In this way the expectation values of the bare electron-jellium potential and the associated spin-orbit contribution are given by

$$\langle\phi_{\mathbf{k},\alpha}|\,\delta W(\mathbf{r})\,|\phi_{\mathbf{k}-\mathbf{q},\alpha}\rangle=M_{\mathbf{q}}A_{\mathbf{q}}, \tag{21}$$

$$\langle\phi_{\mathbf{k},\beta}|\,\delta W_{s\text{-}o}(\mathbf{r})\,|\phi_{\mathbf{k}-\mathbf{q},\alpha}\rangle=M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}A_{\mathbf{q}}, \tag{22}$$

respectively. In order to obtain an explicit expression for the bare matrix elements $M_{\mathbf{q}}$ and $M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}$, we identify the wave functions $\phi_{\mathbf{k},\beta}(\mathbf{r})$ with plane waves, i.e., $\phi_{\mathbf{k},\beta}(\mathbf{r})=e^{i\mathbf{k}\cdot\mathbf{r}}\chi_\beta/\sqrt{V}$, where χ_β is the spinor vector. This leads to

$$M_{\mathbf{q}}=-i\hat{\boldsymbol{\epsilon}}_{\mathbf{q}}\cdot\mathbf{q}\frac{Z_c e^2 n_0}{q^2}, \tag{23}$$

$$M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}=i\frac{\hbar^2}{4m^2c^2}(\mathbf{q}\times\mathbf{k}\cdot\boldsymbol{\sigma}_{\beta\alpha})M_{\mathbf{q}}. \tag{24}$$

In the above equation $\boldsymbol{\sigma}_{\beta\alpha}$ is a short notation for $\chi^{+}_{\beta}\boldsymbol{\sigma}\chi_{\alpha}$. The corresponding screened matrix elements $\hat{M}_{\mathbf{q}}$ and $\hat{M}_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}$ are obtained by using $\delta\widetilde{W}(\mathbf{r})$ and $\delta\widetilde{W}_{s\text{-}o}(\mathbf{r})$ instead of $\delta W(\mathbf{r})$ and $\delta W_{s\text{-}o}(\mathbf{r})$, respectively. In terms of the bare and dressed matrix elements, Eqs. (18) and (19) can be rewritten as

$$\hat{M}_{\mathbf{q}}=M_{\mathbf{q}}+\frac{4\pi e^2}{q^2}2\sum_{\mathbf{k}'}\frac{n_{\mathbf{k}'-\mathbf{q}}-n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}'-\mathbf{q}}-\epsilon_{\mathbf{k}'}}\hat{M}_{\mathbf{q}}, \tag{25}$$

$$\hat{M}_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}=M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}+\frac{\hbar^2}{4m^2c^2}i(\mathbf{q}\times\mathbf{k}\cdot\boldsymbol{\sigma}_{\beta\alpha})\times\frac{4\pi e^2}{q^2}2\sum_{\mathbf{k}'}\frac{n_{\mathbf{k}'-\mathbf{q}}-n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}'-\mathbf{q}}-\epsilon_{\mathbf{k}'}}\hat{M}_{\mathbf{q}}. \tag{26}$$

Equation (25) can be rewritten in the form

$$\hat{M}_{\mathbf{q}}=\frac{M_{\mathbf{q}}}{1+4\pi e^2\chi(\mathbf{q})/q^2}, \tag{27}$$

where $\chi(\mathbf{q})$ is the static limit of the density-density susceptibility in the Lindhard approximation,

$$\chi(\mathbf{q})=-2\sum_{\mathbf{k}}\frac{n_{\mathbf{k}-\mathbf{q}}-n_{\mathbf{k}}}{\epsilon_{\mathbf{k}-\mathbf{q}}-\epsilon_{\mathbf{k}}}. \tag{28}$$

This permits us to write the dressed PMSOI matrix element in the following way:

$$\hat{M}_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}=M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}-\frac{\hbar^2}{4m^2c^2}i(\mathbf{q}\times\mathbf{k}\cdot\boldsymbol{\sigma}_{\beta\alpha})\frac{4\pi e^2}{q^2}\chi(\mathbf{q})\hat{M}_{\mathbf{q}}. \tag{29}$$

By making use of Eqs. (24) and (27), we find

$$\hat{M}_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}=\frac{M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}}{1+4\pi e^2\chi(\mathbf{q})/q^2}. \tag{30}$$

For small momentum transfer $4\pi e^2\chi(\mathbf{q})=k_s^2$ where k_s is the Thomas-Fermi screening momentum,[10] and in this limit $\hat{M}_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}\propto(q/k_s)^2$. This result agrees formally with that of Refs. 2 and 3. However, we would like to stress that Eq. (30) is the result of taking into account the relativistic spin-other-orbits interaction in the calculation of the screening effect. When this interaction is neglected, the PMSOI remains unscreened, and its matrix element is equal to the bare one in Eq. (24).

C. Hartree approximation in the diagrammatic language

We find it useful to translate our result into Feynman's diagrammatic language. This permits us to single out the set of contributions which leads to the screened PMSOI matrix element (30). Moreover, the use of diagrams will enable us to extend easily the present results for the jellium case to those of lattice systems. To this end, we write the total Hamiltonian H as the sum of the free-particle Hamiltonian H_0 and contributions arising from the bare EPI, the bare PMSOI, the Coulomb repulsion H_C and the spin-other-orbits potential $H_{s\text{-}o}$. In the second quantization formalism, we obtain the following interacting Hamiltonians:

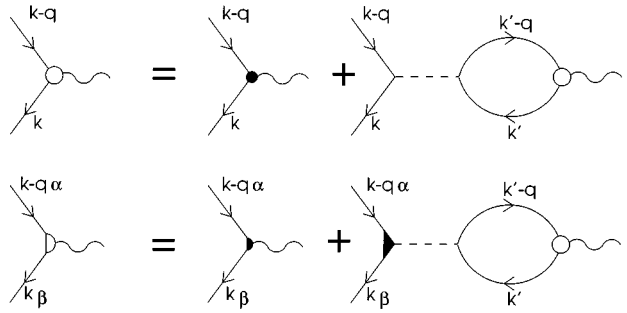

FIG. 1. Dyson equations for the screening of the EPI and PMSOI in the random-phase approximation. Solid lines are the Green's functions for the electron, the wavy lines are phonon propagators. The dashed lines represent the Coulomb repulsion, while a dashed line with a black triangle at one vertex is the spin-other-orbits electron-electron interaction. The dressed EPI matrix element is represented by an open circle while the bare EPI is indicated with a black circle. The empty and full semicircles are the dressed and bare PMSOI matrix elements, respectively. The Greek letters indicate spin indices.

$$H_{\mathrm{EPI}}=\sum_{\mathbf{pq},\alpha}\left(\frac{\hbar}{2MN\omega_{\mathbf{q}}}\right)^{1/2}M_{\mathbf{q}}c^{\dagger}_{\mathbf{k},\alpha}c_{\mathbf{k}-\mathbf{q},\alpha}(b_{\mathbf{q}}+b^{\dagger}_{-\mathbf{q}}), \tag{31}$$

$$H_{\mathrm{PMSOI}}=\sum_{\mathbf{pq},\alpha\beta}\left(\frac{\hbar}{2MN\omega_{\mathbf{q}}}\right)^{1/2}M_{\mathbf{k}\beta,\mathbf{k}-\mathbf{q}\alpha}c^{\dagger}_{\mathbf{k},\beta}c_{\mathbf{k}-\mathbf{q},\alpha}\times(b_{\mathbf{q}}+b^{\dagger}_{-\mathbf{q}}), \tag{32}$$

$$H_C=\tfrac{1}{2}\sum_{\mathbf{kk}'\mathbf{q},\alpha\beta}\frac{4\pi e^2}{q^2}c^{\dagger}_{\mathbf{k},\alpha}c^{\dagger}_{\mathbf{k}',\beta}c_{\mathbf{k}'+\mathbf{q},\beta}c_{\mathbf{k}-\mathbf{q},\alpha}, \tag{33}$$

$$H_{s\text{-}o}=i\frac{e^2\hbar^2}{4m^2c^2}\sum_{\mathbf{kk}'\mathbf{q},\alpha\beta\gamma}\frac{4\pi e^2}{q^2}(\mathbf{q}\times\mathbf{k}\cdot\boldsymbol{\sigma}_{\beta\alpha})\times c^{\dagger}_{\mathbf{k},\beta}c^{\dagger}_{\mathbf{k}',\gamma}c_{\mathbf{k}'+\mathbf{q},\gamma}c_{\mathbf{k}-\mathbf{q},\alpha}. \tag{34}$$

Here $c^{\dagger}_{\mathbf{k},\alpha}(c_{\mathbf{k},\alpha})$ is the creation (annihilation) electron operator for wave number $\mathbf{k}$ and spin state α, $b^{\dagger}_{\mathbf{q}}(b_{\mathbf{q}})$ is the creation (annihilation) operator for phonons with momentum $\mathbf{q}$ and frequency $\omega_{\mathbf{q}}$. In Eqs. (31) and (32), $M_{\mathbf{q}}$ and $M_{\mathbf{k}\alpha,\mathbf{k}-\mathbf{q}\beta}$ are the bare EPI and PMSOI matrix elements given by Eqs. (23) and (24), respectively.

Making use of perturbation theory, we can draw the diagrams which in the static approximation lead to the self-consistent equations (25) and (26). These are shown in Fig. 1, which define a random-phase approximation for the EPI and PMSOI in the presence of the spin-other-orbits electron-electron interaction. The rules for constructing diagrams are the usual ones,[11] and in our notation the full circles and semicircles are the bare EPI and PMSOI matrix elements, respectively, while the dressed quantities are depicted by the corresponding empty symbols. The solid lines refer to electronic Green's functions, and the wavy lines to phonon propagators. The Coulomb interaction $4\pi e^2/q^2$ is represented by a dashed line, and the spin-other-orbits interaction

is composed by a dashed line (which represents the Coulomb interaction) and a black triangle which represent the vertex $i(e^2\hbar^2/4m^2c^2)(\mathbf{q}\times\mathbf{k}\cdot\boldsymbol{\sigma}_{\beta\alpha})$.

The diagrammatic equations in Fig. 1 permit us to generalize the theory of screening of the PMSOI also to the case of a discrete lattice model. In fact, as we shall see in Sec. III, a slightly different reinterpretation of the symbols in Fig. 1 will be sufficient in order to obtain the screened PMSOI matrix element for the lattice model.

III. LATTICE MODEL

A. Bare PMSOI matrix element

An important difference between the jellium model and any other model in which the discrete nature of the lattice is taken into account is the fact that, even for the equilibrium configuration of the lattice, the conduction electrons experience a spin-orbit interaction with the ions. Its strength depends on the penetration of the electronic wave function inside the core region of the ion. As first pointed out by Elliott,[3] this gives rise to an extra contribution to the PMSOI. As we shall see in the following, the screening mechanism of the so-called Elliott's mechanism differs from the one studied in Sec. II.

If we denote with $W(\mathbf{r},\{\mathbf{R}\})$ the bare electron-ion potential for the equilibrium configuration $\{\mathbf{R}\}$ of the ion's position, then the periodic part of the electronic Hamiltonian is[4]

$$H_0=\frac{p^2}{2m}+U(\mathbf{r},\{\mathbf{R}\}), \tag{35}$$

where

$$U(\mathbf{r},\{\mathbf{R}\})=W(\mathbf{r},\{\mathbf{R}\})+\frac{\hbar}{4m^2c^2}\boldsymbol{\nabla}_{\mathbf{r}}W(\mathbf{r},\{\mathbf{R}\})\times\mathbf{p}\cdot\boldsymbol{\sigma}. \tag{36}$$

The second term on the right-hand side of Eq. (36) is the spin-orbit coupling between the conduction electrons and the ions. Because of this term, the eigenfunctions of H_0 are linear combinations of Bloch states of different spins and, neglecting the band index, they can be written in full generality as follows:[3,4]

$$\psi_{\mathbf{k}\uparrow}(\mathbf{r})=\frac{1}{\sqrt{V}}\sum_{\mathbf{Q}}\ (a_{\mathbf{k}+\mathbf{Q}}\chi_\uparrow+b_{\mathbf{k}+\mathbf{Q}}\chi_\downarrow)e^{i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}}. \tag{37}$$

Here $\chi_\uparrow$ and $\chi_\downarrow$ are the spinor vectors with eigenvalues $+1$ and -1 along a given direction and $\mathbf{Q}$ is a vector of the reciprocal lattice. The set of the $b_{\mathbf{k}+\mathbf{Q}}$ functions is proportional to the spin-orbit coupling and it is usually referred to as the small spin component, whereas the coefficients $a_{\mathbf{k}+\mathbf{Q}}$ give rise to the large component. We label the wave function in Eq. (37) with a spinlike quantum number $\uparrow$, but, because of the spin-orbit coupling, it does not correspond to a pure spin state.

The properties of the wave function (37) depend on the symmetry of the Hamiltonian (35). In particular, H_0 is invariant under the time-reversal transformation K which changes the sign of the momentum and spin, leaving the position $\mathbf{r}$ unchanged. Given a state ϕ, then $K\phi$ is called the Kramer conjugate of ϕ. Two important properties of the time-reversal operator are that $K^2=-1$ and, given any two states ϕ and ψ, $\langle\phi|\psi\rangle=\langle K\psi|K\phi\rangle$. It is straightforward to show that the scalar product between any state ϕ and its Kramer conjugate $K\phi$ is zero. In fact, $\langle\phi|K\phi\rangle=\langle K^2\phi|K\phi\rangle=-\langle\phi|K\phi\rangle$. Therefore if ϕ is an eigenstate of H_0, then $K\phi$ is also one and the two are degenerate and orthogonal.

For lattices with inversion symmetry, the Hamiltonian (35) is invariant under a transformation J which transform $\mathbf{r}$ into $-\mathbf{r}$ and $\mathbf{p}$ into $-\mathbf{p}$, leaving the spin $\boldsymbol{\sigma}$ unchanged. In the following we assume that H_0 commutes with J.

Another important transformation is that of conjugation C defined by $C=KJ=JK$. The effect of C is therefore to change the signs of $\boldsymbol{\sigma}$ and $\mathbf{r}$. Also in this case the Hamiltonian H_0 remains invariant (provided that $[H_0,J]=0$). Moreover $C\phi_{\mathbf{k},\uparrow}\propto\phi_{\mathbf{k},\downarrow}$ and $\langle\phi_{\mathbf{k}\uparrow},C\phi_{\mathbf{k}\uparrow}\rangle=0$ because, as in the case of K, $C^2=-1$ and $\langle\phi|\psi\rangle=\langle C\psi|C\phi\rangle$. This can be explicitly seen by applying the operation C on Eq. (37):[12]

$$\psi_{\mathbf{k}\downarrow}(\mathbf{r})=\frac{1}{\sqrt{V}}\sum_{\mathbf{Q}}\ (a^*_{\mathbf{k}+\mathbf{Q}}\chi_\downarrow-b^*_{\mathbf{k}+\mathbf{Q}}\chi_\uparrow)e^{i(\mathbf{k}+\mathbf{Q})\cdot\mathbf{r}}. \tag{38}$$

Small deviations $\mathbf{u}(\mathbf{R})$ from the equilibrium lattice configuration lead to a modulation of both the electron-ion potential and the associated spin-orbit coupling:

$$H_{e\text{-}i}=\sum_{\mathbf{R}}\ \mathbf{u}(\mathbf{R})\cdot\boldsymbol{\nabla}_{\mathbf{R}}U(\mathbf{r},\{\mathbf{R}\}). \tag{39}$$

Because we are interested in the long-range behavior of the unscreened electron-lattice interaction, it is a reasonable approximation to consider a rigid-ion model for the lattice potential. Therefore we define $W(\mathbf{r},\{\mathbf{R}\})=\Sigma_{\mathbf{R}}V(\mathbf{r}-\mathbf{R})$, where $V(\mathbf{r}-\mathbf{R})$ is the potential at position $\mathbf{r}$ generated by the ion at site $\mathbf{R}$. Equation (39) therefore becomes

$$H_{e\text{-}i}=-\sum_{\mathbf{R}}\ \mathbf{u}(\mathbf{R})\cdot\boldsymbol{\nabla}_{\mathbf{R}}\Big[V(\mathbf{r}-\mathbf{R})+\frac{\hbar}{4m^2c^2}\boldsymbol{\nabla}_{\mathbf{r}}V(\mathbf{r}-\mathbf{R})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]. \tag{40}$$

Making use of the set of electronic wave functions (37) and (38), and expanding the displacement vector $\mathbf{u}(\mathbf{R})$ in normal coordinates, $H_{e\text{-}i}$ may be written in the second-quantization representation as follows:

$$\begin{aligned}H_{e\text{-}i}&=H_{\mathrm{EPI}}+H_{\mathrm{PMSOI}}\\&=\sum_{\mathbf{k},\mathbf{q},\lambda}\sum_{\alpha}\left(\frac{\hbar}{2MN\omega_{\mathbf{q},\lambda}}\right)^{1/2}M^{\lambda}_{\mathbf{k},\mathbf{k}-\mathbf{q}}c^{\dagger}_{\mathbf{k},\alpha}c_{\mathbf{k}-\mathbf{q},\alpha}\\&\quad\times(b_{\mathbf{q},\lambda}+b^{\dagger}_{-\mathbf{q},\lambda})+\sum_{\mathbf{k},\mathbf{q},\lambda}\sum_{\alpha,\beta}\left(\frac{\hbar}{2MN\omega_{\mathbf{q},\lambda}}\right)^{1/2}\\&\quad\times M^{\lambda}_{\mathbf{k}\alpha,\mathbf{k}-\mathbf{q}\beta}c^{\dagger}_{\mathbf{k},\alpha}c_{\mathbf{k}-\mathbf{q},\beta}(b_{\mathbf{q},\lambda}+b^{\dagger}_{-\mathbf{q},\lambda}).\end{aligned} \tag{41}$$

Here α and β are spinlike states indices, while λ is the phonon polarization. Furthermore, $M^{\lambda}_{\mathbf{k},\mathbf{k}-\mathbf{q}}$ and $M^{\lambda}_{\mathbf{k}\alpha,\mathbf{k}-\mathbf{q}\beta}$ are the bare EPI and PMSOI matrix elements, respectively. Let us restrict our analysis to the transverse component of the

PMSOI matrix element, which results from a scattering process in which the electron changes its dominant spin state from $\downarrow$ to $\uparrow$:

$$M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=-\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}\langle\psi_{\mathbf{k}\uparrow}|\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot\boldsymbol{\nabla}_{\mathbf{R}}\Big[V(\mathbf{r}-\mathbf{R})+\frac{\hbar}{4m^2c^2}\times\boldsymbol{\nabla}_{\mathbf{r}}V(\mathbf{r}-\mathbf{R})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle. \tag{42}$$

In his work, Overhauser[2] studied only the contribution due to the last term of Eq. (42), whereas Elliott[3] realized that also the first term, the ordinary electron-lattice interaction, can give spin-flip by way of connecting the large and small components of the two spinors [see Eqs. (37) and (38)]. Yafet embodied both approaches by analyzing both terms in Eq. (42). Unlike our approach, he treated the single-ion potential $V(\mathbf{r})$ as an already screened short-ranged potential. In this case the Fourier components of V($\mathbf{r}$) are finite at small $\mathbf{q}$, and it is possible to perform a Taylor expansion of $V(\mathbf{q})$ in power of $\mathbf{q}$. Following this procedure, Yafet was able to demonstrate that the first two terms of the series $M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}\downarrow}+\boldsymbol{\nabla}M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}\downarrow}\cdot\mathbf{q}+\cdots$ vanish. But in our analysis, the potential $V(\mathbf{r})$ is the bare one; therefore its Fourier transform behaves like $V(\mathbf{q})\sim 1/q^2$ for small momentum transfer, and a Taylor expansion of $V(\mathbf{q})$ in powers of $\mathbf{q}$ is not possible. On the other hand, we still can follow to some extent Yafet's elegant procedure by isolating the long-range part of $V(\mathbf{r})$. To this end we write the Fourier transform of $V(\mathbf{r})$ as follows:

$$V(\mathbf{r})=\sum_{\mathbf{q}} V(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}=\sum_{\mathbf{q}}{}'\sum_{\mathbf{G}} V(\mathbf{q}+\mathbf{G})e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}, \tag{43}$$

where $\mathbf{G}$ is a vector of the reciprocal lattice, and the prime means that the summation over $\mathbf{q}$ has to be restricted to the first Brillouin zone. We define $V=V^L+V^S$, where

$$V^L(\mathbf{r})=\sum_{\mathbf{q}}{}' V(\mathbf{q})e^{i\mathbf{q}\cdot\mathbf{r}}, \tag{44}$$

$$V^S(\mathbf{r})=\sum_{\mathbf{q}}{}'\sum_{\mathbf{G}\neq 0} V(\mathbf{q}+\mathbf{G})e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}. \tag{45}$$

While V^L behaves as $1/r$ for long distances, V^S goes faster to zero as $r\to\infty$. We shall see that the latter term satisfies the requirements for the use of Yafet's procedure, whereas V^L leads to a matrix element which can be easily evaluated. Before starting the calculations, we note that in terms of the definitions of V^L and V^S, the periodic part of the Hamiltonian, Eqs. (35) and (36), becomes

$$H_0=\frac{p^2}{2m}+U^S(\mathbf{r},\{\mathbf{R}\}), \tag{46}$$

$$U^S(\mathbf{r},\{\mathbf{R}\})=\sum_{\mathbf{R}}\Big[V^S(\mathbf{r}-\mathbf{R})+\frac{\hbar}{4m^2c^2}\boldsymbol{\nabla}_{\mathbf{r}}V^S(\mathbf{r}-\mathbf{R})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]. \tag{47}$$

In writing Eq. (46), we have left out the infinite constant $NV(0)=\lim_{\mathbf{q}\to 0}NV(\mathbf{q})$. In fact, because of the charge neutrality of the system, this term is canceled by a contribution opposite in sign due to the infinite electrostatic potential generated by the electrons.

By means of Eqs. (44) and (45), the bare PMSOI matrix element can be written as $M=M^S+M^L$, where

$$M^{\lambda,S(L)}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=-\sum_{\mathbf{R}} e^{i\mathbf{q}\cdot\mathbf{R}}\langle\psi_{\mathbf{k}\uparrow}|\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot\boldsymbol{\nabla}_{\mathbf{R}}\Big[V^{S(L)}(\mathbf{r}-\mathbf{R})+\frac{\hbar}{4m^2c^2}\boldsymbol{\nabla}_{\mathbf{r}}V^{S(L)}(\mathbf{r}-\mathbf{R})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle. \tag{48}$$

Let us first consider the term M^S. If we restrict the momenta transfer $\mathbf{q}$ to the first Brillouin zone (we are interested in the limit of small $\mathbf{q}$ only), it is straightforward to show that

$$M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=iN\sum_{\mathbf{G}\neq 0}\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot(\mathbf{q}+\mathbf{G})V(\mathbf{q}+\mathbf{G})\langle\psi_{\mathbf{k}\uparrow}|e^{i(\mathbf{q}+\mathbf{G})\cdot\mathbf{r}}\times\Big[1+\frac{i\hbar}{4m^2c^2}(\mathbf{q}+\mathbf{G})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle. \tag{49}$$

The summation over the reciprocal-lattice vectors $\mathbf{G}$ does not include the value $\mathbf{G}=\mathbf{0}$, and therefore the divergency of $V(\mathbf{q})$ for $\mathbf{q}\to 0$ is removed, and M^S is well defined in the limit of zero momentum transfer. As pointed out previously, we can apply Yafet's method to this term. We therefore perform the $\mathbf{q}\to\mathbf{0}$ limit and transform the result back to real space. In this way we obtain

$$\begin{aligned}M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}\downarrow}&=-\langle\psi_{\mathbf{k}\uparrow}|\hat{\boldsymbol{\epsilon}}_{q,\lambda}\cdot\sum_{\mathbf{R}}\boldsymbol{\nabla}_{\mathbf{R}}\Big[V^S(\mathbf{r}-\mathbf{R})+\frac{\hbar}{4m^2c^2}\times\boldsymbol{\nabla}_{\mathbf{r}}V^S(\mathbf{r}-\mathbf{R})\times\mathbf{p}\cdot\boldsymbol{\sigma}\Big]|\psi_{\mathbf{k}\downarrow}\rangle\\&=-\langle\psi_{\mathbf{k}\uparrow}|\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot\boldsymbol{\nabla}_{\mathbf{r}}U^S(\mathbf{r},\{\mathbf{R}\})|\psi_{\mathbf{k}\downarrow}\rangle,\end{aligned} \tag{50}$$

where $U^S(\mathbf{r},\{\mathbf{R}\})$ is given by Eq. (47). The last equality in the above equation comes from the translational invariance. With the help of Eq. (46), we can therefore write

$$M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}\downarrow}=-\frac{i}{\hbar}\langle\psi_{\mathbf{k}\uparrow}|\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot[\mathbf{p},H_0]|\psi_{\mathbf{k}\downarrow}\rangle. \tag{51}$$

If we denote with $\mathcal{S}$ the operator inside the brackets, and realize that $C\mathcal{S}C^{-1}=\mathcal{S}$, where C is the conjugation operator, then it follows that $\langle\psi_{\mathbf{k}\uparrow}|\mathcal{S}\psi_{\mathbf{k}\downarrow}\rangle=\langle\psi_{\mathbf{k}\uparrow}|\mathcal{S}C\psi_{\mathbf{k}\uparrow}\rangle=\langle C\mathcal{S}C\psi_{\mathbf{k}\uparrow}|\psi_{\mathbf{k}\uparrow}\rangle=-\langle\psi_{\mathbf{k}\uparrow}|\mathcal{S}\psi_{\mathbf{k}\downarrow}\rangle$. Therefore $M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}\downarrow}=0$. By a further application of Yafet's analysis, it is also possible to show that $M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}$ is actually proportional to the second power of q, and, as we shall see in the following, in the small momentum transfer limit this term can be neglected with respect to $M^{\lambda,L}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}$.

Next we make use of the expression of V^L given by Eq. (44), and evaluate the matrix element $M^{\lambda,L}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}$. Performing the summation over $\mathbf{R}$, we obtain

$$M^{\lambda,L}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=iN\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot\mathbf{q}V(\mathbf{q})\Big[\langle\psi_{\mathbf{k}\uparrow}|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle + \frac{i\hbar}{4m^2c^2}\langle\psi_{\mathbf{k}\uparrow}|e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{q}\times\mathbf{p}\cdot\boldsymbol{\sigma}|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle\Big]. \quad (52)$$

Making use of the electronic wave functions (37) and (38), we can evaluate the two terms within the brackets in the limit $\mathbf{q}\rightarrow 0$. Since the second term is already proportional to the small quantity α^2, we consider only the contributions coming from the large spin components in the electronic wave functions. This leads to the result

$$\langle\psi_{\mathbf{k}\uparrow}|e^{i\mathbf{q}\cdot\mathbf{r}}\mathbf{q}\times\mathbf{p}\cdot\boldsymbol{\sigma}|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle=\langle\psi_{\mathbf{k}\uparrow}|\mathbf{q}\times\mathbf{p}\cdot\boldsymbol{\sigma}|\psi_{\mathbf{k}\downarrow}\rangle =\hbar\sum_{\mathbf{Q}}(a^*_{\mathbf{k}+\mathbf{Q}})^2[\mathbf{q}\times(\mathbf{k}+\mathbf{Q})]_+ . \quad (53)$$

Here we used the notation $[\mathbf{v}]_+=v_x-iv_y$, where $\mathbf{v}$ is an arbitrary vector, and v_x and v_y are its components along the x and y axes. For small momentum transfer, the first term within brackets in Eq. (52) also makes a linear contribution in $\mathbf{q}$. In terms of the representations (37) and (38) for the wave functions, this becomes

$$\langle\psi_{\mathbf{k}\uparrow}|e^{i\mathbf{q}\cdot\mathbf{r}}|\psi_{\mathbf{k}-\mathbf{q}\downarrow}\rangle=\sum_{\mathbf{Q}}(b^*_{\mathbf{k}+\mathbf{Q}}a^*_{\mathbf{k}-\mathbf{q}+\mathbf{Q}}-a^*_{\mathbf{k}+\mathbf{Q}}b^*_{\mathbf{k}-\mathbf{q}+\mathbf{Q}}) \sim\mathbf{D}_{\mathbf{k}}\cdot\mathbf{q}, \quad (54)$$

where

$$\mathbf{D}_{\mathbf{k}}=\sum_{\mathbf{Q}}(a^*_{\mathbf{k}+\mathbf{Q}}\boldsymbol{\nabla}_{\mathbf{k}}b^*_{\mathbf{k}+\mathbf{Q}}-b^*_{\mathbf{k}+\mathbf{Q}}\boldsymbol{\nabla}_{\mathbf{k}}a^*_{\mathbf{k}+\mathbf{Q}}). \quad (55)$$

By collecting the results given in Eqs. (52)–(55), we finally obtain the general expression for the transverse component of the bare PMSOI matrix element:

$$M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=M^{\lambda,L}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}+M^{\lambda,S}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow} =iN\hat{\boldsymbol{\epsilon}}_{\mathbf{q},\lambda}\cdot\mathbf{q}V(\mathbf{q})\Big[\mathbf{D}_{\mathbf{k}}\cdot\mathbf{q}+\frac{i\hbar^2}{4m^2c^2}\sum_{\mathbf{Q}}(a^*_{\mathbf{k}+\mathbf{Q}})^2 \times[\mathbf{q}\times(\mathbf{k}+\mathbf{Q})]_+\Big]+\mathcal{O}(q^2). \quad (56)$$

Because $V(\mathbf{q})\sim 1/q^2$, M^S vanishes faster than M^L for $\mathbf{q}\rightarrow\mathbf{0}$, and in the range of $\mathbf{q}$ values of interest for us, we can neglect this contribution. We note moreover, that $\lim_{\mathbf{q}\rightarrow 0}M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}\neq 0$. Qualitatively the same result was obtained in Sec. II for the bare PMSOI matrix element in the jellium model [see Eq. (24)].

B. Screening

Once we have obtained an expression for the bare PMSOI matrix element which includes Elliott's and Overhauser's mechanisms [the first and second terms within the brackets in Eq. (56), respectively], we have to consider the modifications induced by the screening effect of the conduction electrons. From the results obtained in the analysis of the jellium model, it is clear that the screening of the Overhauser part of the PMSOI (which has the same physical origin of the PMSOI in the jellium model) can be achieved by considering the spin-other-orbits electron-electron interaction. We evaluate therefore the matrix element of the potential in Eq. (10) by making use of the electronic wave functions (37) and (38). Within second quantization, the spin-other-orbit interaction takes the form

$$i\frac{\hbar^2}{4m^2c^2}\sum_{\mathbf{k}\mathbf{k}'\mathbf{q},\gamma}\frac{4\pi e^2}{q^2}\sum_{\mathbf{Q}}(a^*_{\mathbf{k}+\mathbf{Q}})^2[\mathbf{q}\times(\mathbf{k}+\mathbf{Q})]_+ \times c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{\mathbf{k}',\gamma}c_{\mathbf{k}'+\mathbf{q},\gamma}c_{\mathbf{k}-\mathbf{q},\downarrow}. \quad (57)$$

Here we have considered only the contribution in which an electron changes its dominant spin state from $\downarrow$ to $\uparrow$, as in the spin-flip transition appearing in Eq. (56). The above result was obtained in the limit of long wavelength, and we have dropped all the terms proportional to the small spin component, because to leading order this expression is already of order α^2.

The spin-other-orbits interaction is able to provide for the screening of the Overhauser part of the PMSOI. But the screening of Elliott's mechanism is of different origin. Because this contribution to the PMSOI comes from a mixing of the small and large spin components of the electronic wave functions, we expect that a similar mixing can be provided by the Coulomb repulsion when wave functions (37) and (38) are used in the calculation of the Coulomb matrix element. This leads to an additional interaction, which in fact can provide the screening of Elliott's term in the PMSOI. The use of wave functions (37) and (38) also leads to terms in which both electrons change their dominant spin state. However, we shall neglect these terms because they do not lead to screening. We therefore consider only terms in which one electron changes its dominant spin state. In the limit of small momentum transfer $\mathbf{q}$, and making use of $\Sigma_{\mathbf{Q}}(|a_{\mathbf{k}+\mathbf{Q}}|^2+|b_{\mathbf{k}+\mathbf{Q}}|^2)=1$ (normalization condition), we obtain the following result:

$$\sum_{\mathbf{k}\mathbf{k}'\mathbf{q},\gamma}\mathbf{D}_{\mathbf{k}}\cdot\mathbf{q}\frac{4\pi e^2}{q^2}c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{\mathbf{k}',\gamma}c_{\mathbf{k}'+\mathbf{q},\gamma}c_{\mathbf{k}-\mathbf{q},\downarrow}, \quad (58)$$

where the vector $\mathbf{D}_{\mathbf{k}}$ is defined in Eq. (55). We write down a generalized spin-other-orbits interaction Hamiltonian, $H^{e\text{-}e}_{s\text{-}o}$, which is defined as the sum of the terms appearing in Eqs. (57) and (58):

$$H^{e\text{-}e}_{s\text{-}o}=\sum_{\mathbf{k}\mathbf{k}'\mathbf{q},\gamma}V_{s\text{-}o}(\mathbf{k}\uparrow,\mathbf{k}'\gamma;\mathbf{k}-\mathbf{q}\downarrow,\mathbf{k}'+\mathbf{q}\gamma) \times c^{\dagger}_{\mathbf{k},\uparrow}c^{\dagger}_{\mathbf{k}',\gamma}c_{\mathbf{k}'+\mathbf{q},\gamma}c_{\mathbf{k}-\mathbf{q},\downarrow}, \quad (59)$$

where

$$V_{s\text{-}o}(\mathbf{k}\uparrow,\mathbf{k}'\gamma;\mathbf{k}-\mathbf{q}\downarrow,\mathbf{k}'+\mathbf{q}\gamma) =\frac{4\pi e^2}{q^2}\Big[\mathbf{D}_{\mathbf{k}}\cdot\mathbf{q}+i\frac{\hbar^2}{4m^2c^2}\sum_{\mathbf{Q}}(a^*_{\mathbf{k}+\mathbf{Q}})^2[\mathbf{q}\times(\mathbf{k}+\mathbf{Q})]_+\Big]. \quad (60)$$

At this point we have all the ingredients for the evaluation of the screened PMSOI matrix element in the long-wavelength

limit. We can make use of the Dyson equation for the response of the electrons to the PMSOI and EPI shown diagrammatically in Fig. 1. This equation was obtained for the jellium model but, with a different reinterpretation of the symbols appearing in Fig. 1, we can also extend its validity to the present case. The full semicircle in Fig. 1 now represents the bare PMSOI matrix element, including both the Overhauser and Elliott terms [Eq. (56)]. The dashed line is still the Coulomb repulsion $4\pi e^2/q^2$, whereas the dashed line attached to a solid triangle represents the generalized spin-other-orbits interaction given by Eq. (60). Therefore, in the static limit the screened PMSOI matrix element $\hat{M}^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}$ satisfies the following equation

$$\hat{M}^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}+\sum_{\mathbf{k}'\gamma}\frac{n_{\mathbf{k}'-\mathbf{q}}-n_{\mathbf{k}'}}{\epsilon_{\mathbf{k}'-\mathbf{q}}-\epsilon_{\mathbf{k}'}}\times V_{s\text{-}o}(\mathbf{k}\uparrow,\mathbf{k}'\gamma;\mathbf{k}-\mathbf{q}\downarrow,\mathbf{k}'+\mathbf{q}\gamma)\hat{M}^{\lambda}_{\mathbf{k}',\mathbf{k}'-\mathbf{q}}, \tag{61}$$

where $\hat{M}^{\lambda}_{\mathbf{k},\mathbf{k}-\mathbf{q}}$ is the screened EPI matrix element. In the long-wavelength limit, it depends only on the momentum transfer $\mathbf{q}$, and it is formally given by Eq. (27), with the bare EPI matrix element approximated by[6]

$$M^{\lambda}_{\mathbf{k},\mathbf{k}-\mathbf{q}}\simeq M^{\lambda}_{\mathbf{q}}=iN\hat{\epsilon}_{\mathbf{q},\lambda}\cdot\mathbf{q}V(\mathbf{q}). \tag{62}$$

By making use of Eq. (60) and the expression for the bare PMSOI given in Eq. (56), from Eq. (61) we obtain

$$\hat{M}^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=\frac{M^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}}{1+4\pi e^2\chi(\mathbf{q})/q^2}. \tag{63}$$

The above result demonstrates that for the lattice case the screening of the PMSOI is given by two mechanisms. The Overhauser contribution is screened by the spin-other-orbits interaction, whereas Elliott's term of the PMSOI is screened by considering the spin-mixing matrix element of the electron-electron Coulomb potential. Moreover, in accordance with Yafet's result,[4] we find that in the limit $\mathbf{q}\rightarrow 0$ the resulting screened PMSOI matrix element, Eq. (63), is proportional to q^2. Because the small spin component of the electronic wave function is of order Δg, the quantity $\mathbf{D}_{\mathbf{k}}$ in Eq. (55) is of order $\Delta g/k_F$, where is the Fermi momentum.[3] Therefore, for materials in which Δg is larger than the fine-structure constant, we can neglect the Overhauser contribution and retain only Elliott's part of the PMSOI. In this way Eq. (63) can be rewritten as

$$\hat{M}^{\lambda}_{\mathbf{k}\uparrow,\mathbf{k}-\mathbf{q}\downarrow}=\hat{M}^{\lambda}_{\mathbf{q}}\mathbf{D}_{\mathbf{k}}\cdot\mathbf{q}\simeq(\Delta g)\hat{M}^{\lambda}_{\mathbf{q}}\frac{q}{k_F}, \tag{64}$$

where we have neglected the angular dependence. The above expression can be used to estimate the PMSOI contribution to T_1^{-1} and it gives a result in accordance with the Elliott-Yafet expression.

IV. CONCLUSIONS

The nature of the screening of the phonon-modulated spin-orbit interaction in metals has been investigated within the Hartree approximation. We have found that the inclusion of relativistic corrections to the electron-electron interaction can provide for a screening of the PMSOI. In particular, the spin-other-orbits interaction is responsible for the screening of Overhauser's term while the screening of the Elliott part of the PMSOI is obtained from the spin-mixing terms in the matrix element of the Coulomb electron-electron repulsion. Finally we have obtained an explicit expression for the screened PMSOI matrix element in the long-wavelength approximation. This is in qualitative agreement with the result of previous theories, which were based on an *a priori* screened lattice potential.[4] Our work provides, therefore, a justification of the already known results and confirms, from a theoretical point of view, the validity of the Elliott-Yafet formula for the electron-spin-relaxation time.

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